Amendments to the Claims:

This listing of claims will replace all prior versions, and listings, of claims in this application.

Listing of Claims:

1-22. (cancelled)

23. (currently amended) A method for selecting a chemical entity that associates with all or part of a binding pocket of a molecule or molecular complex, or a homologue of said binding pocket, with a deformation energy not greater than about 10 kcal/mole, wherein the structure coordinates of inosine monophosphate dehydrogenase ~~("IMPDH")~~ (IMPDH) amino acids 68, 69, 93, 273, 274, 275, 276, 277, 303, 322, 324, 325, 326, 327, 328, 330, 331, 332, 333, 334, 337, 339, 340, 364, 413, 414, 415, 416, 420, 439, 440, 441, 442, 469, and 470 according to Figure 1 characterize the binding pocket, and wherein the homologue of said binding pocket has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å, comprising the steps of:

a)   determining structure coordinates of ~~inosine monophosphate dehydrogenase ("IMPDH")~~ IMPDH amino acids 68,

69, 93, 273, 274, 275, 276, 277, 303, 322, 324, 325, 326, 327, 328, 330, 331, 332, 333, 334, 337, 339, 340, 364, 413, 414, 415, 416, 420, 439, 440, 441, 442, 469, and 470 according to Figure 1 to characterize the binding pocket;

b) employing computational means which utilize all or part of said structure coordinates and structure coordinates of the chemical entity, to dock the chemical entity with all or part of said binding pocket or homologue thereof;

c) quantifying the deformation energy between the chemical entity and all or part of the binding pocket or homologue thereof;

d) outputting said quantified deformation energy to a suitable output hardware; and

e) selecting the chemical entity if said deformation energy is not greater than about 10 kcal/mole.

24-26. (cancelled)

27. (currently amended) A method for selecting a chemical entity that associates with all or part of a binding pocket of a molecule or molecular complex, or a homologue of said binding pocket, with a deformation energy not greater

than about 10 kcal/mole, wherein structure coordinates of

inosine monophosphate dehydrogenase (IMPDH) ~~IMPDH~~ amino acids

275, 276, 303, 325, 326, 331, 333 and 441 according to Figure

1 characterize the binding pocket, and wherein the homologue

of said binding pocket has a root mean square deviation from

the backbone atoms of said amino acids of not more than 1.5 Å,

comprising the steps of:

a)   determining structure coordinates of IMPDH

amino acids 275, 276, 303, 325, 326, 331, 333 and 441

according to Figure 1 to characterize the binding pocket;

b)   employing computational means which utilize all

or part of said structure coordinates and structure

coordinates of the chemical entity, to dock the chemical

entity with all or part of said binding pocket or homologue

thereof;

c)   quantifying the deformation energy between the

chemical entity and all or part of the binding pocket or

homologue thereof;

d)   outputting said quantified deformation energy

to a suitable output hardware; and

e)   selecting the chemical entity if said

deformation energy is not greater than about 10 kcal/mole.

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28. (currently amended) A method for selecting a chemical entity that associates with all or part of a binding pocket of a molecule or molecular complex, or a homologue of said binding pocket, with a deformation energy not greater than about 10 kcal/mole, wherein structure coordinates of inosine monophosphate dehydrogenase (IMPDH) ~~IMPDH~~ amino acids 274, 275, 276, 277, 303, 322, 324, 325, 326, 331, 333, 414, 415, and 441 according to Figure 1 characterize the binding pocket, and wherein the homologue of said binding pocket has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å, comprising the steps of:

a)   determining structure coordinates of IMPDH amino acids 274, 275, 276, 277, 303, 322, 324, 325, 326, 331, 333, 414, 415, and 441 according to Figure 1 to characterize the binding pocket;

b)   employing computational means which utilize all or part of said structure coordinates and structure coordinates of the chemical entity, to dock the chemical entity with all or part of said binding pocket or homologue thereof;

c)   quantifying the deformation energy between the chemical entity and all or part of the binding pocket or homologue thereof;

d)   outputting said quantified deformation energy

to a suitable output hardware; and

e)   selecting the chemical entity if said

deformation energy is not greater than about 10 kcal/mole.

29. (currently amended)   A method for selecting a

chemical entity that associates with all or part of a binding

pocket of a molecule or molecular complex, or a homologue of

said binding pocket, with a deformation energy not greater

than about 10 kcal/mole, wherein the structure coordinates of

inosine monophosphate dehydrogenase ("IMPDH") (IMPDH) amino

acids 67, 68, 69, 70, 73, 274, 275, 276, 303, 322, 323, 324,

325, 326, 327, 328, 329, 330, 331, 332, 333, 334, 335, 364,

365, 366, 367, 368, 385, 386, 387, 388, 389, 391, 411, 412,

413, 414, 415, 416, 419, 440, 441, 442, 443, 500, 501, 502,

503, 504, 505, and 506 according to Figure 1 characterize the

binding pocket, and wherein the homologue of said binding

pocket has a root mean square deviation from the backbone

atoms of said amino acids of not more than 1.5 Å, comprising

the steps of:

a)   determining structure coordinates of inosine

monophosphate dehydrogenase ("IMPDH") IMPDH amino acids 67,

68, 69, 70, 73, 274, 275, 276, 303, 322, 323, 324, 325, 326,

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327, 328, 329, 330, 331, 332, 333, 334, 335, 364, 365, 366,

367, 368, 385, 386, 387, 388, 389, 391, 411, 412, 413, 414,

415, 416, 419, 440, 441, 442, 443, 500, 501, 502, 503, 504,

505, and 506 according to Figure 1 to characterize the binding

pocket;

b)   employing computational means which utilize all

or part of said structure coordinates and structure

coordinates of the chemical entity, to dock the chemical

entity with all or part of said binding pocket or homologue

thereof;

c)   quantifying the deformation energy between the

chemical entity and all or part of the binding pocket or

homologue thereof;

d)   outputting said quantified deformation energy

to a suitable output hardware; and

e)   selecting the chemical entity if said

deformation energy is not greater than about 10 kcal/mole.

30. (currently amended)   A method for selecting a

chemical entity that associates with all or part of a binding

pocket of a molecule or molecular complex, or a homologue of

said binding pocket, with a deformation energy not greater

than about 10 kcal/mole, wherein structure coordinates of

inosine monophosphate dehydrogenase (IMPDH) ~~IMPDH~~ amino acids

68, 70, 322, 328, 329, 331, 332, 335, 364, 366, 387, 388, 411,

413, 414, 415, 441, 442, 501, and 502 according to Figure 1

characterize the binding pocket, and wherein the homologue of

said binding pocket has a root mean square deviation from the

backbone atoms of said amino acids of not more than 1.5 Å,

comprising the steps of:

  a) determining structure coordinates of IMPDH

amino acids 68, 70, 322, 328, 329, 331, 332, 335, 364, 366,

387, 388, 411, 413, 414, 415, 441, 442, 501, and 502 according

to Figure 1 to characterize the binding pocket;

  b) employing computational means which utilize all

or part of said structure coordinates and structure

coordinates of the chemical entity, to dock the chemical

entity with all or part of said binding pocket or homologue

thereof;

  c) quantifying the deformation energy between the

chemical entity and all or part of the binding pocket or

homologue thereof;

  d) outputting said quantified deformation energy

to a suitable output hardware; and

  e) selecting the chemical entity if said

deformation energy is not greater than about 10 kcal/mole.

31. (currently amended)   A method for selecting a
chemical entity that associates with all or part of a binding
pocket of a molecule or molecular complex, or a homologue of
said binding pocket, with a deformation energy not greater
than about 10 kcal/mole, wherein structure coordinates of
inosine monophosphate dehydrogenase (IMPDH) IMPDH amino acids
68, 69, 70, 303, 322, 326, 327, 328, 329, 330, 331, 332, 333,
335, 364, 365, 366, 367, 385, 386, 387, 388, 411, 413, 414,
415, 416, 419, 441, 442, 443, 501, 502, 503, and 504 according
to Figure 1 characterize the binding pocket, and wherein the
homologue of said binding pocket has a root mean square
deviation from the backbone atoms of said amino acids of not
more than 1.5 Å comprising the steps of:

a)   determining structure coordinates of IMPDH
amino acids 68, 69, 70, 303, 322, 326, 327, 328, 329, 330,
331, 332, 333, 335, 364, 365, 366, 367, 385, 386, 387, 388,
411, 413, 414, 415, 416, 419, 441, 442, 443, 501, 502, 503,
and 504 according to Figure 1 to characterize the binding
pocket;

b)   employing computational means which utilize all
or part of said structure coordinates and structure
coordinates of the chemical entity, to dock the chemical

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entity with all or part of said binding pocket or homologue

thereof;

       c)   quantifying the deformation energy between the

chemical entity and all or part of the binding pocket or

homologue thereof;

       d)   outputting said quantified deformation energy

to a suitable output hardware; and

       e)   selecting the chemical entity if said

deformation energy is not greater than about 10 kcal/mole.

       32. (currently amended) A method for selecting a

chemical entity that associates with all or part of a binding

pocket of a molecule or molecular complex, or a homologue of

said binding pocket, with a deformation energy not greater

than about 10 kcal/mole, wherein the structure coordinates of

inosine monophosphate dehydrogenase ~~("IMPDH")~~ (IMPDH) amino

acids 67, 68, 69, 70, 73, 93, 273, 274, 275, 276, 277, 303,

322, 323, 324, 325, 326, 327, 328, 329, 330, 331, 332, 333,

334, 335, 337, 339, 340, 364, 365, 366, 367, 368, 385, 386,

387, 388, 389, 391, 411, 412, 413, 414, 415, 416, 419, 420,

439, 440, 441, 442, 443, 469, 470, 500, 501, 502, 503, 504,

505, and 506 according to Figure 1 characterize the binding

pocket, and wherein the homologue of said binding pocket has a

root mean square deviation from the backbone atoms of said

amino acids of not more than 1.5 Å, comprising the steps of:

a) determining structure coordinates of ~~inosine~~

~~monophosphate dehydrogenase ("IMPDH")~~ IMPDH amino acids 67,

68, 69, 70, 73, 93, 273, 274, 275, 276, 277, 303, 322, 323,

324, 325, 326, 327, 328, 329, 330, 331, 332, 333, 334, 335,

337, 339, 340, 364, 365, 366, 367, 368, 385, 386, 387, 388,

389, 391, 411, 412, 413, 414, 415, 416, 419, 420, 439, 440,

441, 442, 443, 469, 470, 500, 501, 502, 503, 504, 505, and 506

according to Figure 1 to characterize the binding pocket;

b) employing computational means which utilize all

or part of said structure coordinates and structure

coordinates of the chemical entity, to dock the chemical

entity with all or part of said binding pocket or homologue

thereof;

c) quantifying the deformation energy between the

chemical entity and all or part of the binding pocket or

homologue thereof;

d) outputting said quantified deformation energy

to a suitable output hardware; and

e) selecting the chemical entity if said

deformation energy is not greater than about 10 kcal/mole.

33. (currently amended) A method for selecting a chemical entity that associates with all or part of a binding pocket of a molecule or molecular complex, or a homologue of said binding pocket, with a deformation energy not greater than about 10 kcal/mole, wherein structure coordinates of inosine monophosphate dehydrogenase (IMPDH) ~~IMPDH~~ amino acids 68, 70, 275, 276, 303, 322, 325, 326, 328, 329, 331, 332, 333, 335, 364, 366, 387, 388, 411, 413, 414, 415, 441, 442, 501, and 502 according to Figure 1 characterize the binding pocket, and wherein the homologue of said binding pocket has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å comprising the steps of:

a) determining structure coordinates of IMPDH amino acids 68, 70, 275, 276, 303, 322, 325, 326, 328, 329, 331, 332, 333, 335, 364, 366, 387, 388, 411, 413, 414, 415, 441, 442, 501, and 502 according to Figure 1 to characterize the binding pocket;

b) employing computational means which utilize all or part of said structure coordinates and structure coordinates of the chemical entity, to dock the chemical entity with all or part of said binding pocket or homologue thereof;

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c)   quantifying the deformation energy between the chemical entity and all or part of the binding pocket or homologue thereof;

d)   outputting said quantified deformation energy to a suitable output hardware; and

e)   selecting the chemical entity if said deformation energy is not greater than about 10 kcal/mole.

34. (currently amended)   A method for selecting a chemical entity that associates with all or part of a binding pocket of a molecule or molecular complex, or a homologue of said binding pocket, with a deformation energy not greater than about 10 kcal/mole, wherein structure coordinates of inosine monophosphate dehydrogenase (IMPDH) ~~IMPDH~~ amino acids 68, 69, 70, 274, 275, 276, 277, 303, 322, 324, 325, 326, 327, 328, 329, 330, 331, 332, 333, 335, 364, 365, 366, 367, 385, 386, 387, 388, 411, 413, 414, 415, 416, 441, 442, 443, 501, 502, 503, and 504 according to Figure 1 characterize the binding pocket, and wherein the homologue of said binding pocket has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å comprising the steps of:

a)   determining structure coordinates of IMPDH

amino acids 68, 69, 70, 274, 275, 276, 277, 303, 322, 324,

325, 326, 327, 328, 329, 330, 331, 332, 333, 335, 364, 365,

366, 367, 385, 386, 387, 388, 411, 413, 414, 415, 416, 441,

442, 443, 501, 502, 503, and 504 according to Figure 1 to

characterize the binding pocket;

b)   employing computational means which utilize all

or part of said structure coordinates and structure

coordinates of the chemical entity, to dock the chemical

entity with all or part of said binding pocket or homologue

thereof;

c)   quantifying the deformation energy between the

chemical entity and all or part of the binding pocket or

homologue thereof;

d)   outputting said quantified deformation energy

to a suitable output hardware; and

e)   selecting the chemical entity if said

deformation energy is not greater than about 10 kcal/mole.

35 and 36. (cancelled)

37. (previously presented)   The method of claim

32, wherein the docking of the chemical entity with all or

part of the binding pocket utilizes shape complementarity or

is followed by molecular dynamics or energy minimization.

38. (previously presented)   The method according

to any one of claims 23, 29 or 32, further comprising the

steps of:

f)   contacting the selected chemical entity with

the molecule or molecular complex; and

g)   selecting the chemical entity that inhibits the

catalytic activity of the molecule or molecular complex.

39. (cancelled)

40. (previously presented)   The method of claim

32, wherein the docking of the chemical entity with all or

part of the binding pocket includes visual inspection on a

computer screen using a computer program capable of generating

a three-dimensional graphical representation of said structure

coordinates and structure coordinates of said chemical entity.

41. (previously presented)   The method according

to claim 23, 27 or 28, further comprising the steps of:

f) repeating steps a) to e) with a second chemical entity that associates with all or another part of said binding pocket, or homologue thereof;

g) optionally, visually inspecting the relationship of the selected first and second chemical entity to each other in relation to the binding pocket or homologue thereof on a computer screen using the three-dimensional graphical representation of the binding pocket or homologue thereof and said selected first and second chemical entity; and

h) assembling the selected first and second chemical entity into a compound or complex that associates with all or part of said binding pocket or homologue thereof by model building.

42 and 43. (cancelled)

44. (previously presented) The method according to claim 29, 30 or 31, further comprising the steps of:

f) repeating steps a) to e) with a second chemical entity that associates with all or another part of said binding pocket, or homologue thereof;

g)   optionally, visually inspecting the

relationship of the selected first and second chemical entity

to each other in relation to the binding pocket or homologue

thereof on a computer screen using the three-dimensional

graphical representation of the binding pocket or homologue

thereof and said selected first and second chemical entity;

and

h)   assembling the selected first and second

chemical entity into a compound or complex that associates

with all or part of said binding pocket or homologue thereof

by model building.

45 and 46. (cancelled)

47. (previously presented)   The method according

to claim 32, 33 or 34, further comprising the steps of:

f)   repeating steps a) to e) with a second chemical

entity that associates with all or another part of said

binding pocket, or homologue thereof;

g)   optionally, visually inspecting the

relationship of the selected first and second chemical entity

to each other in relation to the binding pocket or homologue

thereof on a computer screen using the three-dimensional

graphical representation of the binding pocket or homologue

thereof and said selected first and second chemical entity;

and

h)   assembling the selected first and second

chemical entity into a compound or complex that associates

with all or part of said binding pocket or homologue thereof

by model building.

48-62. (cancelled)

63. (previously presented)   The method of any one

of claims 23, 29 and 32 wherein the method is for selecting a

chemical entity that associates with all or part of a binding

pocket of a molecule or molecular complex with a deformation

energy not greater than about 7 kcal/mole and step e)

comprises selecting the chemical entity if said deformation

energy is not greater than 7 kcal/mole.

64-71. (cancelled)

72.   (currently amended) A method for selecting a

chemical entity that associates with all or part a binding

pocket of a molecule or molecular complex of inosine

monophosphate dehydrogenase ~~("IMPDH")~~ (IMPDH), or a homologue

thereof, with a deformation energy not greater than about 10

kcal/mole, wherein said homologue of said IMPDH binding pocket

has a root mean square deviation from the backbone atoms of

said amino acids of not more than 1.5 Å, comprising the steps

of:

      a)   employing computational means which utilize all

or part of structure coordinates of said binding pocket

defined by IMPDH amino acids 68, 69, 93, 273, 274, 275, 276,

277, 303, 322, 324, 325, 326, 327, 328, 330, 331, 332, 333,

334, 337, 339, 340, 364, 413, 414, 415, 416, 420, 439, 440,

441, 442, 469, and 470 according to Figure 1, and structure

coordinates of the chemical entity, to dock the chemical

entity with all or part of said binding pocket or homologue

thereof;

      b)   quantifying the deformation energy between the

chemical entity and all or part of the binding pocket or

homologue thereof;

      c)   outputting said quantified deformation energy

to a suitable output hardware; and

      d)   selecting the chemical entity if said

deformation energy is not greater than about 10 kcal/mole.

73. (currently amended)   A method for selecting a chemical entity that associates with all or part a binding pocket of a molecule or molecular complex of inosine monophosphate dehydrogenase ~~("IMPDH")~~ (IMPDH), or a homologue thereof, with a deformation energy not greater than about 10 kcal/mole, wherein said homologue of said IMPDH binding pocket has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å, comprising the steps of:

a)   employing computational means which utilize all or part of structure coordinates of said binding pocket defined by IMPDH amino acids 275, 276, 303, 325, 326, 331, 333 and 441 according to Figure 1, and structure coordinates of the chemical entity, to dock the chemical entity with all or part of said binding pocket or homologue thereof;

b)   quantifying the deformation energy between the chemical entity and all or part of the binding pocket or homologue thereof;

c)   outputting said quantified deformation energy to a suitable output hardware; and

d)   selecting the chemical entity if said deformation energy is not greater than about 10 kcal/mole.

74. (currently amended)   A method for selecting a chemical entity that associates with all or part a binding pocket of a molecule or molecular complex of inosine monophosphate dehydrogenase ("IMPDH") (IMPDH), or a homologue thereof, with a deformation energy not greater than about 10 kcal/mole, wherein said homologue of said IMPDH binding pocket has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å, comprising the steps of:

a)   employing computational means which utilize all or part of said binding pocket structure coordinates defined by IMPDH amino acids 274, 275, 276, 277, 303, 322, 324, 325, 326, 331, 333, 414, 415, and 441 according to Figure 1, and structure coordinates of the chemical entity, to dock the chemical entity with all or part of said binding pocket or homologue thereof;

b)   quantifying the deformation energy between the chemical entity and all or part of the binding pocket or homologue thereof;

c)   outputting said quantified deformation energy to a suitable output hardware; and

d)   selecting the chemical entity if said deformation energy is not greater than about 10 kcal/mole.

75. (currently amended) A method for selecting a chemical entity that associates with all or part a binding pocket of a molecule or molecular complex of inosine monophosphate dehydrogenase ("IMPDH") (IMPDH), or a homologue thereof, with a deformation energy not greater than about 10 kcal/mole, wherein said homologue of said IMPDH binding pocket has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å, comprising the steps of:

a)   employing computational means which utilize all or part of structure coordinates of said binding pocket defined by IMPDH amino acids 67, 68, 69, 70, 73, 274, 275, 276, 303, 322, 323, 324, 325, 326, 327, 328, 329, 330, 331, 332, 333, 334, 335, 364, 365, 366, 367, 368, 385, 386, 387, 388, 389, 391, 411, 412, 413, 414, 415, 416, 419, 440, 441, 442, 443, 500, 501, 502, 503, 504, 505, and 506 according to Figure 1, and structure coordinates of the chemical entity, to dock the chemical entity with all or part of said binding pocket or homologue thereof;

b)   quantifying the deformation energy between the chemical entity and all or part of the binding pocket or homologue thereof;

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c)   outputting said quantified deformation energy
to a suitable output hardware; and

d)   selecting the chemical entity if said
deformation energy is not greater than about 10 kcal/mole.

76. (currently amended)   A method for selecting a
chemical entity that associates with all or part a binding
pocket of a molecule or molecular complex of inosine
monophosphate dehydrogenase ~~("IMPDH")~~ (IMPDH), or a homologue
thereof, with a deformation energy not greater than about 10
kcal/mole, wherein said homologue of said IMPDH binding pocket
has a root mean square deviation from the backbone atoms of
said amino acids of not more than 1.5 Å, comprising the steps
of:

a)   employing computational means which utilize all
or part of structure coordinates of said binding pocket
defined by IMPDH amino acids 68, 70, 322, 328, 329, 331, 332,
335, 364, 366, 387, 388, 411, 413, 414, 415, 441, 442, 501,
and 502 according to Figure 1, and structure coordinates of
the chemical entity, to dock the chemical entity with all or
part of said binding pocket or homologue thereof;

b)   quantifying the deformation energy between the chemical entity and all or part of the binding pocket or homologue thereof;

c)   outputting said quantified deformation energy to a suitable output hardware; and

d)   selecting the chemical entity if said deformation energy is not greater than about 10 kcal/mole.

77. (currently amended) A method for selecting a chemical entity that associates with all or part a binding pocket of a molecule or molecular complex of inosine monophosphate dehydrogenase ("IMPDH") (IMPDH), or a homologue thereof, with a deformation energy not greater than about 10 kcal/mole, wherein said homologue of said IMPDH binding pocket has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å, comprising the steps of:

a)   employing computational means which utilize all or part of structure coordinates of said binding pocket defined by IMPDH amino acids 68, 69, 70, 303, 322, 326, 327, 328, 329, 330, 331, 332, 333, 335, 364, 365, 366, 367, 385, 386, 387, 388, 411, 413, 414, 415, 416, 419, 441, 442, 443, 501, 502, 503, and 504 according to Figure 1, and structure

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coordinates of the chemical entity, to dock the chemical

entity with all or part of said binding pocket or homologue

thereof;

b)   quantifying the deformation energy between the

chemical entity and all or part of the binding pocket or

homologue thereof;

c)   outputting said quantified deformation energy

to a suitable output hardware; and

d)   selecting the chemical entity if said

deformation energy is not greater than about 10 kcal/mole.

78. (currently amended) A method for selecting a

chemical entity that associates with all or part of a binding

pocket of a molecule or molecular complex of inosine

monophosphate dehydrogenase ("IMPDH") (IMPDH), or a homologue

thereof, with a deformation energy not greater than about 10

kcal/mole, wherein said homologue of said IMPDH binding pocket

has a root mean square deviation from the backbone atoms of

said amino acids of not more than 1.5 Å, comprising the steps

of:

a)   employing computational means which utilize all

or part of structure coordinates of said binding pocket

defined by IMPDH amino acids 67, 68, 69, 70, 73, 93, 273, 274,

275, 276, 277, 303, 322, 323, 324, 325, 326, 327, 328, 329,

330, 331, 332, 333, 334, 335, 337, 339, 340, 364, 365, 366,

367, 368, 385, 386, 387, 388, 389, 391, 411, 412, 413, 414,

415, 416, 419, 420, 439, 440, 441, 442, 443, 469, 470, 500,

501, 502, 503, 504, 505, and 506 according to Figure 1, and

structure coordinates of the chemical entity, to dock the

chemical entity with all or part of said binding pocket or

homologue thereof;

b)   quantifying the deformation energy between the

chemical entity and all or part of the binding pocket or

homologue thereof;

c)   outputting said quantified deformation energy

to a suitable output hardware; and

d)   selecting the chemical entity if said

deformation energy is not greater than about 10 kcal/mole.

79. (currently amended) A method for selecting a

chemical entity that associates with all or part a binding

pocket of a molecule or molecular complex of inosine

monophosphate dehydrogenase ("IMPDH") (IMPDH), or a homologue

thereof, with a deformation energy not greater than about 10

kcal/mole, wherein said homologue of said IMPDH binding pocket

has a root mean square deviation from the backbone atoms of

said amino acids of not more than 1.5 Å, comprising the steps of:

a)   employing computational means which utilize all or part of structure coordinates of said binding pocket defined by IMPDH amino acids 68, 70, 275, 276, 303, 322, 325, 326, 328, 329, 331, 332, 333, 335, 364, 366, 387, 388, 411, 413, 414, 415, 441, 442, 501, and 502 according to Figure 1, and structure coordinates of the chemical entity, to dock the chemical entity with all or part of said binding pocket or homologue thereof;

b)   quantifying the deformation energy between the chemical entity and all or part of the binding pocket or homologue thereof;

c)   outputting said quantified deformation energy to a suitable output hardware; and

d)   selecting the chemical entity if said deformation energy is not greater than about 10 kcal/mole.

80. (currently amended)   A method for selecting a chemical entity that associates with all or part a binding pocket of a molecule or molecular complex of inosine monophosphate dehydrogenase ~~("IMPDH")~~ (IMPDH), or a homologue thereof, with a deformation energy not greater than about 10

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kcal/mole, wherein said homologue of said IMPDH binding pocket has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å, comprising the steps of:

a)   employing computational means which utilize all or part of structure coordinates of said binding pocket defined by IMPDH amino acids 68, 69, 70, 274, 275, 276, 277, 303, 322, 324, 325, 326, 327, 328, 329, 330, 331, 332, 333, 335, 364, 365, 366, 367, 385, 386, 387, 388, 411, 413, 414, 415, 416, 441, 442, 443, 501, 502, 503, and 504 according to Figure 1, and structure coordinates of the chemical entity, to dock the chemical entity with all or part of said binding pocket or homologue thereof;

b)   quantifying the deformation energy between the chemical entity and all or part of the binding pocket or homologue thereof;

c)   outputting said quantified deformation energy to a suitable output hardware; and

d)   selecting the chemical entity if said deformation energy is not greater than about 10 kcal/mole.

81. (previously presented)   The method of any one of claims 72, 75 and 78, wherein the method is for selecting a

chemical entity that associates with all or part of a binding

pocket of a molecule or molecular complex of IMPDH, or

homologue thereof, with a deformation energy not greater than

about 7 kcal/mole and step d) comprises selecting the chemical

entity if said deformation energy is not greater than 7

kcal/mole.

82. (previously presented)   The method of claim

78, wherein the docking of the chemical entity with all or

part of the binding pocket utilizes shape complementarity or

is followed by molecular dynamics or energy minimization.

83. (previously presented)   The method according

to any one of claims 72, 75 or 78, further comprising the

steps of:

e)   contacting the selected chemical entity with

the molecule or molecular complex; and

f)   selecting the chemical entity that inhibits the

catalytic activity of the molecule or molecular complex.

84. (previously presented)   The method of claim

78, wherein the docking of the chemical entity with all or

part of the binding pocket includes visual inspection on a

computer screen using a computer program capable of generating

a three-dimensional graphical representation of said structure

coordinates and structure coordinates of said chemical entity.

85. (currently amended) [[A]] The method of claim

82, wherein the method is for selecting a chemical entity

wherein the chemical entity is ~~identifying~~ an inosine

monophosphate dehydrogenase (IMPDH) ~~IMPDH~~ inhibitor.~~,~~

~~comprising the steps of:~~

~~a) docking a chemical entity that is a potential~~

~~IMPDH inhibitor with all or part of a binding pocket defined~~

~~by IMPDH amino acids 67, 68, 69, 70, 73, 93, 273, 274, 275,~~

~~276, 277, 303, 322, 323, 324, 325, 326, 327, 328, 329, 330,~~

~~331, 332, 333, 334, 335, 337, 339, 340, 364, 365, 366, 367,~~

~~368, 385, 386, 387, 388, 389, 391, 411, 412, 413, 414, 415,~~

~~416, 419, 420, 439, 440, 441, 442, 443, 469, 470, 500, 501,~~

~~502, 503, 504, 505, and 506 according to Figure 1, wherein the~~

~~docking of the chemical entity with all or part of the binding~~

~~pocket utilizes shape complementarity or is followed by~~

~~molecular dynamics or energy minimization;~~

~~b)   quantifying the deformation energy between the~~

~~chemical entity and all or part of the binding pocket thereof;~~

~~c) outputting said quantified deformation energy~~

~~to a suitable output hardware; and~~

~~d) selecting the chemical entity, and thereby~~

~~identifying the IMPDH inhibitor, if said deformation energy is~~

~~not greater than about 10 kcal/mole.~~